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On the Reconstruction of a Weak Phase-Amplitude Object. I

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Abstract

In this paper we consider the reconstruction of a weak amplitude-phase object. We mean by this reconstruction of the wave function in a plane directly behind the object. The program is carried through with the aid of two measurements of the contrast, corresponding to different values of the defocusing.

Inhalt

Über die Rekonstruktion eines schwachen Phasen-Amplituden-Objekts.I. In diesem Aufsatz betrachten wir die Rekonstruktion eines schwachen Phasen-Amplitudenobjekts. Damit meinen wir die Rekonstruktion der Wellenfunktion in einer Ebene gleich hinter dem Objekt. Das Verfahren wird durchgeführt mittels zweier Kontrastmessungen, welche zwei verschiedenen Werten der Defokussierung entsprechen.

1. Introduction

The purpose of microscopy is to get information about an object. Therefore one lets take place an interaction between the object and an electron wave. Coherent illumination will be assumed. The wave function of the scattered electron on the plane just behind the object (object plane) is transported through the electromagnetic field of an electron microscope and, using the Schrödinger equation one can calculate the wave function on some other plane. After the measurement of an observable quantity, for instance the contrast in the Gaussian image, there arises the question if the object wave function i.e. the wave function just behind the object can be reconstructed from this measurement. If this reconstruction has been performed we have essentially only two dimensional information about the object. This follows from the fact that the object wave function depends upon the projection of the potential distribution describing the object along the direction of the illuminating plane wave [9]. In another paper soon to be published we will show how a three dimensional object reconstruction can be performed if the object is illuminated from different directions. In the first part of the paper we will give a short survey of the theory of ideal image formation, thereby discussing the influence of a diaphragm on the image wave function. This will be done in a novel form, with the use of the spheroidal and G.P.S.F. functions, analysed by *Slepian*, *Pollack* et al. [1] and recently [2, 6] used in treating corresponding problems in light optics. In the second part it will be shown, that, with the aid of two measurements of the contrast, taken at two different adjustments of the defocusing, the object wave function of a weak amplitude-phase object (Zernike-Gabor object) can be reconstructed. Of vital importance, especially in electron optics, is the determination of the influence of aberrations on the imaging process. We therefore take into account the following aberrations, which have the greatest influence on the imaging process, namely:

a) Spherical aberration
b) Defocusing
c) Coma.

In the analysis of the reconstruction problem two cases will be treated separately:

a) Image formation with a rectangular diaphragm
b) Image formation with a circular diaphragm.

For physical reasons one does not expect great differences between these two cases as far as imaging properties are concerned. The mathematical treatment is completely different, however!

2. Image formation by a rectangular diaphragm without aberrations

In this paragraph the propagation of the object wave function will be considered in case of a rectangular diaphragm. To calculate the image wave-function the following three assumptions are made:

a) the image formation is paraxial
b) the calculation of the image wave function can be performed using first order W.K.B. approximation
c) the electromagnetic field is rotationally symmetric.

With these three assumptions *Glaser* (ref. 3, formula (160.34)) has derived the following relation between the wave function in an arbitrary plane $z = z_B$, and the object wave function:

$$g(z_B, x_B, y_B) = \frac{p_0^{3/2}}{2\pi i\hbar t_B (p_B)^{1/2}} \iint_\sigma \psi(z_0, x_0, y_0) \exp\left[\frac{i}{2\hbar t_B} S(x_0, y_0, x_B, y_B)\right] dx_0\, dy_0 \qquad t_B \neq 0 \tag{2.1}$$

where $g(z_B, x_B, y_B)$ is the wave function on the plane $z = z_B$ and $\psi(z_0, x_0, y_0)$ is the wave function on the plane $z = z_0$: the object wave function. z_B is chosen such that $t_B \neq 0$. [We abbreviate $t(z_B)$ by t_B]

$$S(x_0, y_0, x_B, y_B) = p_0 s_B (x_0^2 + y_0^2) - 2p_0(x_0 x_B + y_0 y_B) + p_B t'_B (x_B^2 + y_B^2)$$

p_0 is the classical momentum of an electron at $z = z_0$
p_B is the classical momentum of an electron at $z = z_B$

s(z) and t(z) are two linearly independent solutions of the paraxial ray equation.

$$(\Phi)^{\frac{1}{2}} \frac{d}{dz}\left((\Phi) \frac{d\varrho}{dz}\right) + \tfrac{1}{4}\left(\Phi'' + \frac{e}{2m} B_z^2\right) \varrho = 0 \qquad \text{(ref. 3, formula (160.10))}$$

satisfying the initial conditions: $s(z_0) = 1 \quad t(z_0) = 0$
$s'(z_0) = 0 \quad t'(z_0) = 1$

Φ is the electrostatic potential along the optical axis which is chosen to be the z-axis and B_z is the magnetic induction along the z-axis.

$$s_B = s(z_B); \qquad t_B = t(z_B); \qquad t'_B = \left(\frac{dt}{dz}\right)_{z = z_B} \tag{2.2}$$

From formula (2.3) one derives by letting t_B go to zero the following relationship between the image wave function in a plane $z = z_1$ where $t(z_1) = 0$, and the object wave function:

$$g(z_1, x_1, y_1) = \left(\frac{p_0}{p_B}\right)^{\frac{1}{2}} \frac{1}{s_1} \psi\left(z_0, \frac{x_1}{s_1}, \frac{y_1}{s_1}\right) \exp\left\{\frac{i p_0 s'_1}{2\hbar s_1}(x_1^2 + y_1^2)\right\} \tag{2.3}$$

(ref. 3, formula (161.8))

From formula (2.3) one derives the current density in the plane $z = z_1$, which is proportional to the current density in the object-plane. Therefore, the plane $z = z_1$ will be called the image-plane (Gaussian image). In order to calculate the influence of a diaphragm on this result, formula (2.1) has to be applied twice: once to calculate the wave function in the plane of the diaphragm starting from the known object wave function and once to calculate the wave function in the image-plane, starting from the calculated wave function in the plane of the diaphragm. This last calculation is made with the assumption that the wave function is zero on the opaque part of the diaphragm. According to *Glaser* (ref. 3, formula (161.22)), the following relationship exists between the image- and object wave function:

$$g(z_1, x_1, y_1) = \exp\left[\frac{-i p_1 (s_B t'_1 - t_B s'_1)}{2\hbar s_1 t_B}(x_1^2 + y_1^2)\right] \times$$
$$\times \iint_\sigma K_0(x_1, y_1, x_0, y_0) \exp\left\{\frac{i p_0}{2\hbar t_B} s_B (x_0^2 + y_0^2)\right\} \psi(z_0, x_0, y_0)\, dx_0\, dy_0 \tag{2.4}$$

where

$$K_0(x_1, y_1, x_0, y_0) \tag{2.5}$$
$$= \frac{p_0^2}{4\pi^2 \hbar^2 s_1 t_B^2}\left(\frac{p_0}{p_1}\right)^{\frac{1}{2}} \iint_D \exp\left[\frac{-i p_0}{\hbar t_B}\left\{\left(x_0 - \frac{x_1}{s_1}\right) x_B + \left(y_0 - \frac{y_1}{s_1}\right) y_B\right\}\right] dx_B\, dy_B.$$

D is the aperture of the diaphragm.

In case of a rectangular diaphragm with vertices $\left[\pm\frac{a}{2}; \pm\frac{b}{2}\right]$ the function $K_0(x_1, y_1, x_0, y_0)$ equals:

$$K_0(x_1, y_1, x_0 y_0) = A \int_{-1}^{+1} d\tilde{x}_B \int_{-1}^{+1} d\tilde{y}_B \exp\left\{ i\omega \left(x_0 - \frac{x_1}{s_1} \tilde{x}_B \right) + i\omega' \left(y_0 - \frac{y_1}{s_1} \right) \tilde{y}_B \right\} \tag{2.6}$$

$$A = \frac{p_0^2 ab}{16 \hbar^2 s_1 t_B^2} \left(\frac{p_0}{p_1}\right)^{\frac{1}{2}}; \qquad \omega = \frac{p_0 a}{2\hbar t_B \pi}; \qquad \omega' = \frac{p_0 b}{2\hbar t_B \pi} \tag{2.7}$$

$$\tilde{x}_B = \frac{2x_B}{a}; \qquad \tilde{y}_B = \frac{2y_B}{b} \tag{2.8}$$

For further discussion the function:

$$h(x_0, y_0, z_0) = \psi(x_0, y_0, z_0) \exp\left[\frac{ip_0}{2\hbar t_B} \cdot s_B(x_0^2 + y_0^2) \right] \tag{2.9}$$

is developed into a series of spheriodal functions. These functions form a complete orthonormal system on the interval [—1, +1] and are the eigenfunctions of the following integral equation:

$$\alpha_j^c \varphi_j^c(x) = \int_{-1}^{+1} e^{icxy} \varphi_j^c(y)\, dy \tag{2.10}$$

with orthogonality property:

$$\int_{-1}^{+1} \varphi_j^c(x)\, \varphi_k^c(x)\, dx = \delta_{j,k} \tag{2.11}$$

We assume a rectangular object. With a suitable choice of the units in the object plane we can accomplish that $-1 \leqq x_0 \leqq 1$
$-1 \leqq y_0 \leqq 1$

From the completeness and the orthonormality of the functions $\varphi_j^c(x)$ we may expand $h(x_0, y_0, z_0)$ into the following series

$$h(x_0, y_0, z_0) = \sum_{j,k=0}^{\infty} A_{j,k}(z_0)\, \varphi_j^\omega(x_0)\, \varphi_k^{\omega'}(y_0) \tag{2.12}$$

$\varphi_j^\omega(x_0)$ is an eigenfunction of the integral equation (2.10) with $c = \omega$ and eigenvalue $\alpha^\omega{}_j$
$\varphi_k^{\omega'}(y_0)$ is an eigenfunction of the integral equation (2.10) with $c = \omega'$ and eigenvalue $\alpha^\omega{}_k'$.

$$A_{j,k}(x) = \int_{-1}^{+1} dx_0 \int_{-1}^{+1} dy_0\, h(x_0, y_0, z_0)\, \varphi_j^\omega(x_0)\, \varphi_k^{\omega'}(y_0)$$

Using (2.6), (2.10) and (2.12) one derives from (2.4)

$$g(z_1, x_1, y_1) = \exp\left\{\frac{-ip_1}{2\hbar s_1} \cdot \frac{s_B t'_1 - t_B s'_1}{t_B} (x_1^2 + y_1^2)\right\} \times$$
$$\times A \sum_{j,k=o}^{\infty} (\alpha_j{}^{\omega} \alpha_k{}^{\omega'})^2 A_{j,k}(z_0) \varphi_j{}^{\omega}\left(-\frac{x_1}{s_1}\right) \varphi_k{}^{\omega'}\left(-\frac{y_1}{s_1}\right) \tag{2.13}$$

The eigenvalues have the following asymptotic behaviour for $\omega \to \infty$

$$(\alpha^{\omega}{}_j)^2 = \frac{2\pi}{\omega}\left[1 - \frac{4\pi^{\frac{1}{2}}}{j!} z^{3j} (\omega^{j+1/2} e^{-2\omega})\ 1 + 0\left(\frac{1}{\omega}\right)\right] \quad \text{(See ref. 1)} \tag{2.14}$$

So if the diaphragm is infinite ($a \to \infty$; $b \to \infty$), which means $\omega \to \infty, \omega' \to \infty$, we have from (2.14)

$$\alpha^{\omega}{}_j \approx \frac{2\pi}{\omega}; \qquad \alpha^{\omega'}{}_k \approx \frac{2\pi}{\omega'}; \qquad \text{for each j and k.}$$

Substituting this limiting case in (2.13) and using the relation: $\frac{p_0}{s_1} = p_1 t'_1$ (see ref. 3, form. (160.24) with $t_1 = 0$) we have rederived equation (2.3).

3. Image formation by a circular diaphragm without aberrations

In this paragraph the influence of a circular diaphragm on the image formation will be analysed. We start again from formula (2.4) and assume that the object wave function is zero outside a circular domain of radius 1. The radius of the diaphragm is Ω. Formula (2.4) becomes, after transformation to cylindrical coordinates r_1, Φ_1, z_1:

$$g(r_1, z_1, \Phi_1) =$$
$$\exp\left\{-\frac{ip_1}{2\hbar s_1} \cdot \frac{s_B t'_1 - t_B s'_1}{t_B} r_1^2\right\} \int_0^1 r_0 \, dr_0 \int_0^{2\pi} d\Phi_0$$
$$K_0(r_1, \Phi_1, r_0, \Phi_0)\, \psi(r_0, \Phi_0, z_0) \exp\left\{\frac{ip_0 s_B}{2\hbar t_B} r_0^2\right\} \tag{3.1}$$

where

$$K_0(r_1, \Phi_1, r_0, \Phi_0) =$$
$$= A \int_0^{\Omega} r_B \, dr_B \int_0^{2\pi} d\Phi_B \exp\left[-\frac{ip_0}{\hbar t_B}\left\{r_B r_0 \cos(\Phi_B - \Phi_0) - r_B \frac{r_1}{s_1} \cos(\Phi_B - \Phi_1)\right\}\right] \tag{3.2}$$

With: $\begin{cases} x_B = r_B \cos \Phi_B \\ y_B = r_B \sin \Phi_B \end{cases} \begin{cases} x_0 = r_0 \cos \Phi_0 \\ y_0 = r_0 \sin \Phi_0 \end{cases} \begin{cases} x_1 = r_1 \cos \Phi_1 \\ y_1 = r_1 \sin \Phi_1 \end{cases}$ (3.3)

Introduce furthermore the abbreviations:

$$e = -\frac{p_1}{2\hbar s_1} \cdot \frac{s_B t'_1 - t_B s'_1}{t_B} \tag{3.4}$$

$$d = \frac{p_0}{\hbar t_B} \tag{3.5}$$

In the formula (3.2) we use the following expansion:

$$\exp\{ix \cos \alpha\} = \sum_{n=-\infty}^{+\infty} i^n J_n(x) \exp(i\alpha n) \tag{3.6}$$

(see ref. 5, page 22, where Θ has been replaced by $\Theta + \frac{\pi}{2}$).

Furthermore we expand the image and object wave function in a Fourier series:

$$\psi(r_0, \Phi_0, z_0) = \sum_{n=-\infty}^{+\infty} e^{in\Phi_0} \hat{\varphi}_n(r_0, z_0) \tag{3.7}$$

$$g(r_1, \Phi_1, z_1) = \sum_{l=-\infty}^{+\infty} e^{il\Phi_1} \hat{g}_l(r_1, z_1) \tag{3.8}$$

From (3.1), (3.2), (3.6), (3.7) and (3.8) we get after performing the integrations over Φ_B and Φ_0:

$$\hat{g}_n(r_1, z_1) = A \exp\{ier_1^2\}\, 2\pi\Omega^2 \int_0^1 r_0\, dr_0 \int_0^{\Omega} \tilde{r}_B\, d\tilde{r}_B\, J_n(\Omega \tilde{r}_B d) J_n(\Omega r_0 \tilde{r}_B \frac{r_1}{s_1} d) \times$$
$$\times \hat{\psi}_n(r_0, z_0) \exp\left\{\frac{i}{2} s_B r_0^2 d\right\}. \tag{3.9}$$

where $\tilde{r}_B = \frac{r_B}{\Omega}$, and the following relation has been used:

$$J_{-n}(z) = (-1)^n J_n(z) \tag{3.10}$$

(see ref. 5, page 15, form. 2)

Formula (3.9) shows, that, in case of image formation without aberrations, the n^{th} Fouriercomponent in the image depends only on the n^{th} Fouriercomponent in the object, a result which has been derived in the light optical case by *Toraldo di Francia* [6]. We now proceed analogously as in section 2 and develop the function $\hat{\psi}_n(r_0, z_0) \exp\left(\frac{id}{2} \frac{i}{2} s_B r_0^2 d\right)$ in a series of "Generalised Prolate Spheroidal Functions" (G.P.S.F.). These functions form a complete orthonormal system on the interval [0,1], and are the eigenfunctions of the following integral equation:

$$\lambda_j^c\, p_j^c(r) = \int_0^1 J_n(crr')\, r'\, p_j^c(r')\, dr' \tag{3.11}$$

with orthogonality property:

$$\int_0^1 p_j^c(r')\, p_K^c(r')\, r'\, dr' = \delta_{j,K} \tag{3.12}$$

So we have:

$$\psi_n(r_0, z_0) \exp\left\{\frac{i}{2} s_B r_0^2 d\right\} = \sum_{j=o}^{\infty} B_j(z_0)\, p_j^{\Omega d} \tag{3.13}$$

If (3.13) is inserted in (3.9) and if property (3.11) is applied twice we find the following expression for the n^{th} Fourier component of the image wave function:

$$\hat{g}_n(r_1, z_1) = 2\pi\Omega^2 \sum_{j=0}^{\infty} (\lambda_j^{\Omega d})^2\, B_j(z_0)\, p_j^{\Omega d}\left(\frac{r_1}{s_1}\right) \exp\{ier_1^2\} \tag{3.14}$$

The eigenvalue has the following asymptotic behaviour for $c \to \infty$

$$c^{1/2}\lambda_j^c = \frac{(-1)^j}{c^{1/2}} - \frac{(-1)^j \pi^{2n+4j+2} c^{n+2j+1/2} e^{-2c}}{\Gamma(j+1) \quad \Gamma(j+n+1)} \left[1 + 0\left(\frac{1}{c}\right)\right]$$

(See ref. 1)

So, if $\Omega \gg 1$ we have $\left|\lambda_j^{\Omega d}\, \Omega\right| \approx \frac{1}{d}$, and we have found back the ideal image formation.

Note: In section 1 we have assumed a rectangular object, and in section 2 a circular object. This is, however, no limitation at all, for let the object have any finite form, then one can enclose this object within a rectangle or circle. In that case we define the object wave function as zero on those parts inside the rectangle or circle which lie outside the transparent part of the object plane.

4. Image formation by a rectangular diaphragm with aberrations

Until now, we have considered the image formation without aberrations and looked for the influence of a diaphragm. In the following sections 4 and 5 we will give the corresponding formulae in case the aberrations are taken into account. These formulae will be used to solve the reconstruction problem.

For the analysis of this case we use a formula, derived by *Glaser* (ref. 3, formula (181.22)) which is in fact a generalisation of the formula which was used in sections 2 and 3. Under the three conditions, stated in section 2, the following relationship exists between the wave function of image and object in a plane $z = z_1$, *where we have to restrict ourselves to planes for which* $t(z_1) \neq 0$.

$$g(z_1, x_1, y_1) = \frac{1}{2\pi i\hbar}\left(\frac{p_0}{p_1}\right)^{\frac{1}{2}} \iint_\sigma \left(\frac{p_0}{t_1} + A\varrho + B\chi + CR + D\sigma\right) \times$$
$$\times \exp\left\{\frac{i}{\hbar} S\left(x_0, y_0, x_B, y_B\right)\right\} \psi(z_0, x_0, y_0)\, dx_0\, dy_0 \qquad (4.1)$$

$$S(x_0, y_0, x_1, y_1) = \int_{z_5}^{z_1} p(\tau)\, d\tau + \frac{1}{2t_1}[p_1 t'_1\varrho - 2p_0\chi + p_0 s_1 R] - p_1[\tfrac{1}{4} A_1 R^2 +$$
$$+ \tfrac{1}{4} B_1 \varrho^2 + C_1\chi^2 + \tfrac{1}{2} DR\varrho + E_1 R\chi + F_1\varrho\chi + e_1 R\sigma + c\chi\sigma + f_1\varrho\sigma] \qquad (4.2)$$

$$R = x_0^2 + y_0^2;\ \varrho = x_1^2 + y_1^2;\ \chi = x_0 x_1 + y_0 y_1;\ \sigma = x_0 y_1 - y_0 x_1 \qquad (4.3)$$

A (not to be confused with A in (2.7)), B . . . . D; A_1 . . . . F_1; e_1 . . . . f_1 are the aberration constants which are calculated by integration of certain quantities along the paraxial rays. See *Glaser* (ref. 3, formulae (103.30) and (181.23)).

In the following calculations with this formula, the following two assumptions are made:

a) the image formation is so strongly paraxial that we can neglect in the development of S all those terms which are of higher order than linear in x_0 and y_0.

b) of the aberration coefficients only two are important in (4.1), namely:
B_1: spherical aberration
F_1: coma.

To a certain extent this is made plausible by a numerical calculation of the aberration coefficients performed by *Storbeck* [7] for the case of an immersion-lens. The image wave function will be calculated *under the assumption* $s_B = 0$, which physically means that the diaphragm is in the Fraunhofer plane. With the two assumptions mentioned above, we get, in analogy with the calculation in section 2, by applying formula (4.1) twice (once for the calculation of the wave function in the plane of the diaphragm and once for the calculation of the image wave function), the following relationship between the image and object wave function:

$$g(z_1, x_1, y_1) = \exp\{ier_1^2\} \iint_\sigma K(x_1, y_1, x_0, y_0)\, \psi(x_0, y_0, z_0)\, dx_0\, dy_0 \qquad (4.4)$$

where

$$K(x_1, y_1, x_0, y_0) = \frac{A}{ab}\left(\frac{p_0}{p_1}\right)^{\frac{1}{2}} \int_{-\frac{a}{2}}^{+\frac{a}{2}} dx_B \int_{-\frac{b}{2}}^{+\frac{b}{2}} dy_B \exp\left[id\left\{\left(x_0 - \frac{x_1}{s_1}\right) x_B\right.\right.$$

$$+ \left(y_0 - \frac{y_1}{s_1}\right) y'_B - i\frac{p_1}{\hbar} F_1 (x_B^2 + y_B^2)(x_B x_0 + y_B y_0) \tag{4.5}$$

$$- i\frac{p_1}{\hbar} F'_1 (x_1^2 + y_1^2)(x_1 x_B + y_1 y_B) - i\frac{p_1}{4} B_1(x_B^2 + y_B^2)^2$$

$$\left.\left. - i\frac{p_1}{4} B'_1(x_1^2 + y_1^2)^2 + \frac{\Delta z}{2l^2}(x_B^2 + y_B^2)\right\}\right]$$

l is the object focal distance. Further we introduced the defocusing Δz which is related to $t(z_1)$ by the following formula:

$\dfrac{\Delta z}{2l^2} = \dfrac{p_B s'_B t_1}{2t_B s_1}$ (see ref. 8, formula (37)).

The term $\dfrac{\Delta z}{l2}(x_B^2 + y_B^2)$ arises from the defocusing $(t(z_1) \neq 0)$.

It is convenient to rewrite equation (4.5) as follows:

$$K(x_1, y_1, x_0, y_0) = \frac{A}{ab}\left(\frac{p_0}{p_1}\right)^{\frac{1}{2}} \int_{-\frac{a}{2}}^{+\frac{a}{2}} dx_B \int_{-\frac{b}{2}}^{+\frac{b}{2}} dy_B \exp\left\{i(x_0 X_B + y_0 Y_B) - \right.$$

$$- i(x_B X_1 + y_B Y_1) + i\frac{C_s}{4l^4}(x_B^2 + y_B^2)^2 + \tag{4.6}$$

$$\left. + i\frac{C'_s}{4l^4}(x_1^2 + y_1^2)^2 + i\frac{\Delta z}{2l^2}(x_B^2 + y_B^2)\right\}$$

where we introduced the customary symbols C_s and C'_s according to:

$\dfrac{C_s}{4l^4} = -\dfrac{p_1}{4} B_1$; $\dfrac{C'_s}{4l^4} = -\dfrac{p_1}{4} B'_1$ (see ref. 8, formula (37))

with:

$$\left\{\begin{aligned} X_B &= x_B d - \frac{p_1 F_1}{\hbar}(x_B^2 + y_B^2)\, x_B \\ Y_B &= y_B d - \frac{p_1 F_1}{\hbar}(x_B^2 + y_B^2)\, y_B \end{aligned}\right. \qquad \left\{\begin{aligned} X_1 &= -\frac{x_1}{s_1} d - \frac{p_1 F'_1}{\hbar}(x_1^2 + y_1^2)\, x_1 \\ Y_1 &= -\frac{y_1}{s_1} d - \frac{p_1 F'_1}{\hbar}(x_1^2 + y_1^2)\, y_1 \end{aligned}\right. \tag{4.7}$$

So the influence of the coma can be taken into account by a coordinate transformation in the image plane.

Formula (4.4) gives the relationship between the object and image wave function. However, the wave function itself is not observable, only its modulus. Observable quantities are the current density in the image plane or a related quantity: the contrast of the image. We will concentrate upon the latter. The contrast of an image $C(x_1, y_1, z_1)$ is defined as follows:

$$C(x_1, y_1, z_1) = \frac{|g(x_1, y_1, z_1)|^2 - |\iint_\sigma K(x_1, y_1, x_0, y_0)\, dx_0\, dy_0|^2}{|\iint_\sigma K(x_1, y_1, x_0, y_0)\, dx_0\, dy_0|^2} \tag{4.8}$$

The term

$$\iint_\sigma K(x_1, y_1, x_0, y_0)\, dx_0\, dy_0 \tag{4.9}$$

is the wave function which would be obtained if there were no object. We will assume that our object is a "weak" object, which we will now define more precisely. If we assume an illuminating plane wave the wave function just behind the object is written as

$$\psi(x_0, y_0, z_0) = \exp\{ikz_0\} \cdot \exp\{i\eta(x_0, y_0, z_0) + f(x_0, y_0, z_0)\} \tag{4.10}$$

The expression $\exp\{i\eta + f\}$ is the transmission function of the object and contains information about the structure. Our aim is to reconstruct η and f from the contrast in the observation plane. This procedure becomes managable if we make the simplifying assumption that we are dealing with a weak object $|\eta| \ll 1$

$|f| \ll 1.$

In that case (4.10) may be approximated by

$$\psi(x_0, y_0, z_0) \approx \exp\{ikz_0\}\,(1 + i\eta(x_0, y_0, z_0) + f(x_0, y_0, z_0)) \tag{4.11}$$

From (4.4), (4.6), (4.7), (4.8) and the approximation (4.11) we derive:

$$\begin{aligned} C(x_1, y_1, z_1) = {} & U(x_1, y_1, z_1) \iint_\sigma dx_0\, dy_0 \iint_D dx_B\, dy_B \exp\{i(x_0 X_B + y_0 Y_B - \\ & - x_B X_1 - y_B Y_1)\} \times \\ & \times \{\sin\{W(r_B)\}\, \eta(x_0, y_0, z_0) + \cos\{W(r_B)\}\, f(x_0, y_0, z_0)\} + \\ & + V(x_1, y_1, z_1) \iint_\sigma dx_0\, dy_0 \iint_D dx_B\, dy_B \\ & \times \exp\{i(x_0 X_B + y_0 Y_B - x_B X_1 - y_B Y_1)\} \times \\ & \times \{\cos\{W(r_B)\}\, \eta(x_0, y_0, z_0) \\ & + \sin\{W(r_B)\}\, f(x_0, y_0, z_0)\{\, |\iint_\sigma K(x_1, y_1, x_0, y_0)\, dx_0\, dy_0|^{-2} \end{aligned} \tag{4.12}$$

where

$$\iint_\sigma K(x_1, y_1, x_0, y_0)\, dx_0\, dy_0 = U(x_1, y_1, z_1) + iV(x_1, y_1, z_0); \qquad (4.13)$$

U and V real.

$$W(r_B) = \frac{C_s}{4l^4} r_B^4 + \frac{\Delta z}{2l^2} r_B^2.$$

$W(r_B)$ denotes the well-known expression for phase-shift in the plane of the diaphragm due to spherical aberration and defocusing.

In the derivation of (4.12), explicit use has been made of the assumption that the transmitting part of the diaphragm is symmetric with respect to the optical axis.

We assume $|V(x_1, y_1, z_1)| \ll |U(x_1, y_1, z_1)|$. This is made plausible from the following considerations:

Consider the formula:

$$Y(x_1, y_1, z_1) = U(x_1, y_1, z_1) + i\,V(x_1, y_1, z_1) = \iint_\sigma K(x_1, y_1, x_0, y_0)\, dx_0\, dy_0 \qquad (4.14)$$

This is (4.4) with $s_B = 0$ and with $\psi(z_0, x_0, y_0) = 1$. Form the difference $Y(x_1, y_1, z_1) - Y^*(x_1, y_1, z_1) = 2i\,V(x_1, y_1, z_1)$. Performing the integration over the object plane $z = z_0$, which will now be assumed to be infinite, one derives from (4.14) with (4.6):

$$V(x_1, y_1, z_1) \qquad (4.15)$$
$$= \frac{ab}{A} \iint_\sigma dx_B\, dy_B\, \delta(X_B)\, \delta(Y_B) \exp\{-ix_B X_1 - iy_B Y_1\} \sin\{W(r_B)\}$$

From (4.15) we see that $V(x_1, y_1, z_1)$ would be exactly zero, if the aberrations had not been taken into account, for then $W(r_B) = 0$. So, if we assume that the influence of the aberrations is small enough, the inequality

$$|V(x_1, y_1, z_1)| \ll |U(x_1, y_1 z_1)| \qquad (4.16)$$

is valid.

Consider the operator

$$\Delta = -\left(\frac{\partial^2}{\partial X_1^2} + \frac{\partial^2}{\partial Y_1^2}\right) \qquad (4.17)$$

and its effect on the function $\exp\{-ix_B X_1 - iy_B Y_1\}$

$$\Delta \exp\{-ix_B X_1 - iy_B Y_1\} = (x_B^2 + y_B^2) \exp\{-ix_B X_1 - iy_B Y_1\} \qquad (4.18)$$

So with the assumption (4.16) and the relation (4.18), (4.12) is written for *two* different adjustments of the defocusing. This is necessary for we have to reconstruct two functions (η and f) so we must have two linearly independent equations. These may be written in operator form:

$$U_K(X_1, Y_1, z_1)\, C_K(X_1, Y_1, z_1)$$
$$= \sin\{W_K(\Delta)\} \iint_\sigma K(X_1, Y_1, x_0, y_0)\, \eta(x_0, y_0, z_0)\, dx_0\, dy_0$$
$$+ \cos\{W_K(\Delta)\} \iint_\sigma K(X_1, Y_1, x_0, y_0)\, f(x_0, y_0, z_0)\, dx_0\, dy_0. \tag{4.19}$$

$k = 1,2.$

$$W_K(r_B) = \frac{C_S}{4l^4} r_B^4 + \frac{\Delta z_K}{2l^2} r_B^2$$

$$K(X_1, Y_1, x_0, y_0)$$
$$= \iint_\sigma dx_0\, dy_0 \iint_D dx_B\, dy_B \exp\{i(x_0 X_B + y_0 Y_B - x_B X_1 - y_B Y_1)\} \tag{4.20}$$

The set of equations (4.19) can be considered as a set of linear equations for the unknown functions:

a. $\iint_\sigma K(X_1, Y_1, x_0, y_0)\, \eta(x_0, y_0, z_0)\, dx_0\, dy_0$ (4.21)

b. $\iint_\sigma K(X_1, Y_1, x_0, y_0)\, f(x_0, y_0, z_0)\, dx_0\, dy_0$ (4.22)

from which we can solve them with the aid of Cramer's rule. Symbolical application of this rule gives:

a. $\iint_\sigma K(X_1, Y_1, x_0, y_0)\, \eta(x_0, y_0, z_0)\, dx_0\, dy_0 =$ (a)

$$-\begin{vmatrix} \sin\{W_1(\Delta)\} & \cos\{W_1(\Delta)\} \\ \sin\{W_2(\Delta)\} & \cos\{W_2(\Delta)\} \end{vmatrix}^{-1} \times \begin{vmatrix} \cos\{W_1(\Delta)\} & U_1(X_1, Y_1, z_1)\, C_1(X_1, Y_1, z_1) \\ \cos\{W_2(\Delta)\} & U_2(X_1, Y_1, z_1)\, C_2(X_1, Y_1, z_1) \end{vmatrix}$$

b. $\iint_\sigma K(X_1, Y_1, x_0, y_0)\, f(x_0, y_0, z_0)\, dx_0\, dy_0 =$ (4.23) (b)

$$\begin{vmatrix} \sin\{W_1(\Delta)\} & \cos\{W_1(\Delta)\} \\ \sin\{W_2(\Delta)\} & \cos\{W_2(\Delta)\} \end{vmatrix}^{-1} \times \begin{vmatrix} \sin\{W_1(\Delta)\} & U_1(X_1, Y_1, z_1)\, C_1(X_1, Y_1, z_1) \\ \sin\{W_2(\Delta)\} & U_2(X_1, Y_1, z_1)\, C_2(X_1, Y_1, z_1) \end{vmatrix}$$

The first operator on the righthand side of (4.23a) and (4.23b) has to be understood as the inverse of the operator

$$\begin{vmatrix} \sin\{W_1(\Delta)\} & \cos\{W_1(\Delta)\} \\ \sin\{W_2(\Delta)\} & \cos\{W_2(\Delta)\} \end{vmatrix} \tag{4.24}$$

The justification for this inverse will be given later on.

We will now justify the expression (4.23a). The justification for (4.23b) proceeds in the same way.

Operate with
$\cos\{W_2(\Delta)\}$ on (4.19) with $k = 1$, and with $\cos\{W_1(\Delta)\}$ on (4.19) with $k = 2$

and subtract the two equations, which results in

$$\cos\{W_2(\Delta)\}\, U_1(X_1, Y_1, z_1)\, C_1(X_1, Y_1, z_1)$$
$$-\cos\{W_1(\Delta)\}\, U_2(X_1, Y_1, z_1)\, C_2(X_1, Y_1, z_1)$$
$$= \iint_\sigma dx_0\, dy_0 \iint_D dx_B\, dy_B$$
$$\exp\{i(x_0 X_B + y_0 Y_B - x_B X_1 - y_B Y_1)\}$$
$$\sin\{W_1(r_B) - W_2(r_B)\}\, \eta(x_0, y_0, z_0). \tag{4.25}$$

(4.25) is the ėvaluation of the second factor in the r.h.s. of (4. 23a).

In the following theorem we will now give a precise mathematical definition of the inverse of the operator (4.24).

Theorem:

Let $\varepsilon_0 > 0$. Then there exists a finite set of real numbers d_j such that:

$$\sum_{j=0}^{n} d_j \Delta^j \left[\cos\{W_2(\Delta)\}\, U_1(X_1, Y_1, z_1)\, C_1(X_1, Y_1, z_1)\right.$$
$$\left.-\cos\{W_1(\Delta)\}\, U_2(X_1, Y_1, z_1)\, C_2(X_1, Y_1, z_1)\right]$$
$$= \iint_\sigma K(X_1, Y_1, x_0, y_0)\, \eta(x_0, y_0, z_0)\, dx_0\, dy_0 + \varepsilon_0(X_1, Y_1);$$
$$|\varepsilon_0(X_1, Y_1)| < \varepsilon_0; \text{(for all } X_1, Y_1, \text{ lying in } |X_1| < \infty\ |Y_1| < \infty) \tag{4.26}$$

Proof:

Define the following function $n(r_B)$ (intended as a representation of the inverse of (4.24))

$$n(r_B) = \frac{1}{\sin\{W_1(r_B) - W_2(r_B)\}}$$

if
$$(n-1)\pi + \delta \leqslant W_1(r_B) - W_2(r_B) \leqslant n\pi - \delta$$

$n(r_B)$ is some continuous connection between the points

$$\left(n\pi - \delta, \frac{1}{\sin(n\pi - \delta)}\right) \text{ and } \left(n\pi + \delta, \frac{1}{\sin(n\pi + \delta)}\right)$$

if
$$n\pi - \delta \leqq W_1(r_B) - W_2(r_B) \leqq n\pi + \delta \tag{4.27}$$

δ may be chosen arbitrarily positive.

Let ε_1 be some arbitrarily small positive number. The function $n(r_B)$ can be approximated arbitrarily closely and uniformly in the interval $[0, (a^2 + b^2)^{1/2}]$ by a finite polynomial as stated by a celebrated theorem of *Weierstrasz* (ref. 4, chapter II, §4).

$$n(r_B) = \sum_{j=0}^{n} d_j r_B^{2j} + \varepsilon_1(r_B); \quad |\varepsilon_1(r_B)| < \varepsilon_1 \text{ for } 0 \leqq r_B \leqq (a^2 + b^2)^{1/2} \tag{4.28}$$

From (4.18), (4.25) and (4.28) we derive:

$$\Big| \sum_{j=0}^{n} d_j \Delta^j [\cos\{W_2(\Delta)\}\ U_1(X_1, Y_1, z_1)\, C_1(X_1, Y_1, z_1)$$

$$- \cos\{W_1(\Delta)\}\ U_2(X_1, Y_1, z_1)\, C_2(X_1, Y_1, z_1)]$$

$$- \iint_\sigma K(X_1, Y_1, x_0, y_0)\, \eta(x_0, y_0, z_0)\, dx_0\, dy_0 \Big|$$

$$= \Big| \iint_\sigma dx_0\, dy_0 \iint_D dx_B\, dy_B \exp\{i(x_0 X_B + y_0 Y_B - x_B X_1 - y_B Y_1)\} \times$$

$$\times\, \eta(x_0, y_0, z_0)\, [\{\sin\{W(r_B)\}\}\{n(r_B) + \varepsilon_1(r_B)\} - 1]$$

$$\leqq \iint_\sigma dx_0\, dy_0 \iint_D dx_B\, dy_B\, |\eta(x_0, y_0, z_0)|\ |\varepsilon_1(r_B)|$$

$$+ \sum_{n=0}^{j} \iint_\sigma dx_0\, dy_0 \iint_{W(r_B) = n\pi - \delta}^{W(r_B) = n\pi + \delta} dx_B\, dy_B\ |\sin W(r_B)\, n(r_B)|\ |\eta(x_0, y_0, z_0)|$$

$$\leqq a.b.M.\varepsilon_1 + 2p\delta M$$

M is the maximum of $|\eta(x_0, y_0, z_0)|$ if $|x_0| \leqq 1$, $|y_0| \leqq 1$

p is the number of zero's of

$$\sin\{W_1(r_B) - W_2(r_B)\} \text{ if } |x_B| \leqq \frac{a}{2},\quad |y_B| \leqq \frac{b}{2} \tag{4.29}$$

If we choose $\delta = \dfrac{\varepsilon_0}{4\,pM}$ and $\varepsilon_1 = \dfrac{ab\varepsilon_0}{2}$ the relation (4.26) is proved.

The symbolic solution (4.23a) has now been justified. Completely analogously we derive the following expression:

$$\sum_{j=0}^{n} d_j \Delta^j [\sin\{W_1(\Delta)\}\ U_1(X_1, Y_1, z_1)\, C_1(X_1, Y_1, z_1)$$

$$- \sin\{W_2(\Delta)\}\, U_2(X_1, Y_1, z_1)\, C_2(X_1, Y_1, z_1)]$$

$$= \iint_\sigma K(X_1, Y_1, x_0, y_0)\, f(x_0, y_0, z_0)\, dx_0\, dy_0 + \varepsilon_2(X_1, Y_1). \tag{4.30}$$

$|\varepsilon_2(X_1, Y_1)| < \varepsilon_2$, if ε_2 is some arbitrarily small positive number.

So we have reduced the reconstruction problem to the determination of η and f from the expressions (4.26) and (4.30).

This can be done immediately for inserting the explicit formula (4.20). into (4.26), the right hand side of (4.26) can be rewritten as follows:

$$\iint_\sigma K(X_1, Y_1, x_0\, y_0)\, \eta(x_0, y_0, z_0)\, dx_0\, dy_0$$

$$= \iint_D dx_B\, dy_B \exp\{-i(x_B X_1 + y_B Y_1)\}\ P(X_B, Y_B) \tag{4.31}$$

$$P(X_B, Y_B) = \iint_\sigma dx_0\, dy_0 \exp\{i(x_0 X_B + y_0 Y_B)\}\, \eta(x_0, y_0, z_0). \quad (4.32)$$

So $P(X_B, Y_B)$ is the finite Fourier transform of $\eta(x_0, y_0, z_0)$ and the left hand side of (4.32) is the finite Fourier transform of $P(X_B, Y_B)$. We will prove in the appendix the following theorem: Let h(y) be a real or complex function defined in the interval [—a. +a] and piecewise continuous. Let g(x) be defined by the following expression:

$$g(x) = \int_{-a}^{+a} e^{icxy}\, h(y)\, dy \quad (4.33)$$

and be known in some interval [—b, +b]. Then we can determine h(y) uniquely from the knowledge of g(x) in the interval [—b, +b]. So from the knowledge of the lefthand side of (4.26) we are able to determine $P(X_B, Y_B)$ and from the knowledge of $P(X_B, Y_B)$ we determine $\eta(x_0, y_0, z_0)$. Completely analogous $f(x_0, y_0, z_0)$ is reconstructed from the kowledge of the left hand side of (4.30).

5. Reconstruction for a circular diaphragm

The derivation of the set of equations in the case of a circular diaphragm is analogous with the derivation in the rectangular case, and we get from (3.6), (3.7), (3.8), (4.4), (4.5), (4.8), (4.11) and (4.16):

$$U_k(R_1, z_1)\,{}_k\hat{C}_n(R_1, z_1) = \int_0^1 r_0\, dr_0 \int_0^\Omega r_B\, dr_B\, J_n(r_0 R_B)\, J_n(r_B R_1)\, [\sin\{W_k(r_B)\} \times$$

$$\times\, \hat{n}_n(r_0, z_0) - \cos\{W_k(r_B)\}\, \hat{f}_n(r_0, z_0)] \quad (5.1)$$

for defocusing Δz_k and $k = 1,2$. ${}_k\hat{C}_n$ is the n^{th} Fourier component of the contrast in measurement k

$$R_B = \hbar r_B d - p_1 F_1 r_B^3;\; R_1 = -\hbar \frac{r_1}{s_1} d_1 + \frac{F'_1}{s_1} r_1^3. \quad (5.2)$$

$U_k(R_1, z_1)$ is the real part of the image wave function arising from the incident wave (background wave function) at defocusing Δz_k.

Consider the following operator:

$${}_nO_{R_1} = -R_1^{-n-1} \frac{\partial}{\partial R_1}\left[R_1^{2n+1}\left[\frac{\partial}{\partial R_1} R_1^{-n}\right]\right] \quad (5.3)$$

which has the property:

$${}_nO_{R_1} J_n(r_B R_1) = r_B^2 J_n(r_B R_1) \quad (5.4)$$

We may rewrite (5.1) in operator form:

$$U_k(R_1, z_1)\ {}_k\hat{C}_n(R_1, z_1) = \sin \{W_k({}_nO_{R_1})\}\ H\ \{\hat{n}_n(r_0, z_0)\}$$
$$+ \cos \{W_k({}_nO_{B_1})\}\ H\ \{\hat{f}_n(r_0, z_0)\}\ k = 1{,}2. \tag{5.5}$$

$H\ \{g(r_0)\}$ is defined by:

$$H\ \{g(r_0)\} = \int_0^1 r_0\, dr_0 \int_0^\Omega r_B\, dr_B\, J_n(r_0 R_B)\, J_n(r_B R_1)\, g(r_0) \tag{5.6}$$

With the procedure of section 4 the following equations are derived:

$$\text{a. } H\ \{\hat{n}_n(r_0, z_0)\} = \sum_{j=0}^{n} d_j\ {}_nO^j{}_{R_1} [\cos \{W_2({}_nO_{R_1})\}\ U_1(R_1, z_1)\ {}_1\hat{C}_n(R_1, z_1)$$
$$- \cos \{W_1({}_nO_{R_1})\}\ U_2(R_1, z_1)\ {}_2\hat{C}_n (R_1, z_1)] + \varepsilon_3(r_0)$$

$$\text{b. } H\ \{\hat{f}_n(r_0, z_0)\} = \sum_{j=0}^{n} d_j\ {}_nO^j{}_{R_1} [\sin \{W_1({}_nO_{R_1})\ U_1(R_1, z_1)\ {}_1\hat{C}_n (R_1, z_1)$$
$$-\sin \{W_2({}_nO_{R_1})\}\ U_2(R_1, z_1)\ {}_2\hat{C}_n (R_1, z_1)] + \varepsilon_4(r_0)$$
$$|\varepsilon_3(r_0)| \text{ and } |\varepsilon_4(r_0)| \text{ arbitrarily small}$$
$$\text{for } 0 \leqq r_0 \leqq 1 \tag{5.7}$$

According to the definition (5.6) $H\ \{\hat{n}_n(r_0, z_0)\}$ may be split up as follows:

$$H\ \{\hat{n}(r_0, z_0)\} = \int_0^\Omega r_B\, dr_B\, J_n(r_B R_1)\, Q(R_B) \tag{5.8}$$

$$Q(R_B) = \int_0^1 r_0\, dr_0\, J_n(r_0 R_B)\, \hat{n}_n(r_0). \tag{5.9}$$

The right hand side of (5.8) is the finite Hankel transform of $Q(r_B)$. In the appendix it will be proven that we can reconstruct $Q(r_B)$ in some finite interval from the knowledge of the right hand side of (5.8) in some finite r_0-interval. The same argument can be applied to determine $\hat{n}_n(r_0, z_0)$ in the interval [0,1] from the relation (5.9).

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Appendix

The derivation of an inversion formula for the finite Fourier and Hankel transforms.

Theorem:

Let h(y) be a real or complex function of the real variable y on the interval [—a, +a], which is piecewise continuous on this interval. Let g(x) (x is a real variable) be defined by the following expression:

$$g(x) = \int_{-a}^{+a} e^{icxy}\, h(y)\, dy \tag{A.1}$$

and be known in some interval [—b, +b]. Then can h(y) be determined uniquely from the knowledge of g(x) in the interval [—b, +b].

Proof:

With the substitutions
$$\begin{cases} x = \tilde{x}\, b \\ y = \tilde{y}\, a \end{cases} \tag{A.2}$$

(A.1) is transformed into:

$$g(\tilde{x}\, b) = \int_{-1}^{+1} e^{icab\tilde{x}\tilde{y}}\, ah(a\tilde{y})\, d\tilde{y} \qquad \begin{cases} |\tilde{x}| \leqq 1 \\ |\tilde{y}| \leqq 1 \end{cases} \tag{A.3}$$

We now apply the technique described in section 2. Developing the function a h(a$\tilde{y}$) into a series of spheroidal functions (which are *complete* and orthonormal in the interval [—1, +1]) one obtains

$$\begin{aligned} a\, h(a\tilde{y}) &= \sum_{j=0}^{\infty} A_j (\alpha_j{}^{cab})^{-1} \Phi_j{}^{cab}(\tilde{y}) \\ A_j &= \int_{-1}^{+1} g(\tilde{x}b)\, \Phi_j{}^{cab}(\tilde{x})\, d\tilde{x}. \end{aligned} \tag{A.4}$$

For the finite Hankel transform there exists an analogous theorem:

Theorem:

Let h(y) be a real or complex function of the real variable y on the interval [0, a], which is piecewise continuous on this interval.

Let g(x) (x is a real variable) be defined by the following expression:

$$g(x) = \int_0^a y\, J_n(cxy)\, h(y)\, dy \tag{A.5}$$

and be known in some interval [0, b]. Then h(y) can be determined uniquely from the knowledge of g(x) in the interval [0, b].

Proof:

With the substitutions
$$\begin{aligned} x &= \tilde{x}\, b \\ y &= \tilde{y}\, a \end{aligned}$$

(A.5) is transformed into:

$$g(\tilde{x}b) = \int_0^1 \tilde{y}\, J_n(cab\tilde{x}\tilde{y})\, a^2\, h(a\tilde{y})\, d\tilde{y} \quad \begin{matrix} |\tilde{x}| \leqq 1 \\ |\tilde{y}| \leqq 1 \end{matrix} \tag{A.6}$$

Developing the function $a^2\, h(a\tilde{y})$ into a series of G.P.S.F., see section 3 (which are *complete* and orthonormal in the interval [0,1]) one obtains:

$$a^2\, h(a\tilde{y}) = \sum_{j=0}^{\infty} B_j (\lambda_j^{cab})^{-1}\, p_j^{cab}(\tilde{y}) \tag{A.7}$$

$$B_j = \int_0^1 g(\tilde{x} b)\, p_j^{cab}(\tilde{x})\, d\tilde{x}$$

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